

The Merck Index OnlineSM

FILE DESCRIPTION

The Merck Index OnlineSM is the online version of the monographs in the printed 12th Edition of *The Merck Index* (a U.S. publication, Whitehouse Station, N.J., USA), an internationally recognized, one-volume encyclopedia of chemicals, drugs, and biologicals. Each monograph in the encyclopedia (each record in the database) discusses a single chemical entity or a small group of very closely-related compounds. Updates contain material not yet available in print.

Records contain molecular formulas and weights, systematic chemical names (including CAS names), generic and trivial names, brand names and their associated companies, company codes, CAS Registry numbers, physical and toxicity data, therapeutic and commercial uses, and bibliographic citations to the chemical, biomedical, and patent literature.

SUBJECT COVERAGE

The database includes, but is not limited to, monographs on the following types of compounds:

- Agricultural chemicals (including pesticides and herbicides)
- Biological products
- Environmentally significant compounds
- Human drugs
- Natural products
- Organic and inorganic chemicals used in commerce and research
- Veterinary drugs

SOURCES

Records contain information from and citations to approximately 700 international chemical, biomedical, and clinical journals; patents issued by more than 20 countries; books; proceedings; and other standard reference works.

DIALOG FILE DATA

Inclusive Dates: Late 19th Century to the present

Update Frequency: Semi-Annual

File Size: 10,430 records as of February 1998

CONTACT

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File 304
SAMPLE RECORD

The Merck Index OnlineSM

AN=/MN,MN=/DE,/NA,NA=/MAIN

RN=

MF=, MW=

/CN, CN=, /NA, NA=, /DE

/SY, SY=, /NA, NA=, /DE

/SO, SO=

PN=
/DERIV

/SY, SY=, /NA, NA=, /DE

RN=

MF=

/SY, SY=, /NA, NA=, /DE
/TN, TN=, /SY, SY=,
/NA, NA=, /DE

/CO, CO=

/PP, PP=

MP=, MT=
OP=, OT=

/SY, SY=, /NA, NA=, /DE
/TN, TN=, /SY, SY=, /NA,

NA=, /DE

/CO, CO=

/TC, TC=

/TC, TV=

/DP, RP=

/DP, DP=

/DP, DP=, /DERIV

DIALOG(R)File 304:The Merck Index Online(SM)
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03605 Monograph Name: Enalapril

CAS REGISTRY NUMBER: 75847-73-3

MOLECULAR FORMULA: C20H28N2O5 MOLECULAR WEIGHT: 376.45

MOLECULAR COMPOSITION: C 63.81%, H 7.50%, N 7.44%, O 21.25%

C.A. CHEMICAL NAME(s): (S)-1-(N-(1-(Ethoxycarbonyl)-3-phenylpropyl)-L-alanyl)-L-proline
SYNONYMS:

1-(N-((S)-1-carboxy-3-phenylpropyl)-L-alanyl)-L-proline 1'-ethyl ester
LITERATURE REFERENCES:

Angiotensin-converting enzyme (ACE) inhibitor; de-esterified in vivo to its active diacid metabolite, enalaprilat, q.v. Prepn: A. Patchett et al., Nature 288, 280 (1980); eidem, Eur. pat. Appl. 12,401; E. E. Harris et al., U.S. pat. 4,374,829 (1980, 1983 both to Merck & Co.). Pharmacology: D. M. Gross et al., J. Pharmacol. Exp. Ther. 216, 552 (1981); C. S. Sweet et al., ibid. 558. Bioavailability and metabolism: E. H. Ulm, Drug Metab. Rev. 14, 99 (1983). Comprehensive description: D. P. Ip, G. S. Brenner, Anal. Profiles Drug Subs. 16, 207-243 (1987). Clinical trial in congestive heart failure: Consensus Trial Study Group, N. Engl. J. Med. 316, 1429 (1987). Review of clinical experience in hypertension: H. J. Gomez et al., J. Cardiovasc. Pharmacol. 15, Suppl. 3, S26-S29 (1990); of clinical pharmacokinetics: R. J. MacFadyen et al., Clin. Pharmacokinet. 25, 274-282 (1993); of combination with hydrochlorothiazide: P. L. Malini, Adv. Ther. 10, 253-262 (1993).

PATENT INFORMATION:

EP 12401; US 4374829

DERIVATIVE INFORMATION:

SUBSTANCE: Enalapril Maleate

DERIVATIVE CAS RN: 76095-16-4

DERIVATIVE MOL. FORMULA: C20H28N2O5.C4H4O4

DERIVATIVE DRUG CODES: MK-421

DERIVATIVE BRAND NAME (COMPANY): Amprace (Amrad), Bitensil (UCB), Cardiovet (Intervet), Enacard (Merck & Co.), Enaloc (Leiras), Enapren (Merck & Co.), Glioten (Bago), Hipoartel (Lasa), Innovace (Merck & Co.), Lotrial (Roemmers), Olivin (Lek), Pres (Dieckmann), Renitec (Merck & Co.), Reniten (Merck & Co.), Renivace (Banyu), Vasotec (Merck & Co.), Xanef (Merck & Co.)
DERIVATIVE PHYSICAL DATA: White to off-white crystalline powder, mp 143-144.5 degrees. Solv (g/ml): water 0.025; alcohol 0.08; methanol 0.20. (.alpha.)D25 -42.2 degrees (c = 1 in methanol). pH (1% water) 2.6. pKa1 3.0; pKa2 (25 degrees) 5.4.

MELTING POINT: 143-144.5 degrees

OPTICAL ROTATION: (.alpha. D): -42.2 degrees (c = 1 in methanol)

SUBSTANCE: Enalapril Mixture of maleate with hydrochlorothiazide

DERIVATIVE BRAND NAME (COMPANY): Acesistem (Sigma-Tau), Co-Renitec (Merck & Co.), Innozide (Merck & Co.), Renacor (Merck & Co.), Vaseretic (Merck & Co.), Xynertec (Merck & Co.)

THERAPEUTIC CATEGORY: Antihypertensive.

THERAPEUTIC CATEGORY VET: In treatment of heart failure in dogs.

REFERENCE KEYS PRESENT: Clinical trial; In Vivo; Patent number;

Pharmacology; Prepn; Review

DATA KEYS PRESENT: Molecular weight; Patent number; Therap. Cat.; Therap. Cat. Vet.

DATA KEYS PRESENT IN DERIVATIVE: Melting point; Optical rotation

SEARCH OPTIONS

BASIC INDEX

SEARCH SUFFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
—/CN	—/CN	All Basic Index Fields CA Chemical Name ^{1,2}	Word Segment & Word & Phrase	S ETHOXCARBONYL(1W)PHENYLPROPYL S PROPYL/CN S
/CO/DE	CO DE	Company Name ¹ Chemical Name	Word Segment & Word & Phrase	ETHOXCARBONYL(1W)PHENYLPROPYLCN S "S)-1-(N-(1-(ETHOXCARBONYL)-3"?/CN S MERCK/CO S PHENYL/DE
/DP/EC/MN	DP MF MN	Data Present ^{1,3} Element Count ² Monograph Name ¹	Word Phrase Segment & Word & Phrase	S ENALAPRIL(W)MALEATE/DE S ENALAPRIL MALEATE/DE S MELTING(W)POINT S (C20(S)N2)/EC S CHLORIDE/MN S ENALAPRIL/MN S ANTIMONY TRICHLORIDE/MN S PHENYL/NA
/NA	NA	Chemical Name ¹	Segment & Word & Phrase	S ENALAPRIL(W)MALEATE/NA S ENALAPRIL MALEATE/NA
/NT/PP/SO	NT PP SO	Notes and Cautions Physical Property Information ³ Sources/References ⁴	Word Word Word	S MORDANT(S)CATALYST/NT S WHITE(1W)POWDER/PP S ACADEMIC(W)PRESS/SO S U(W)S(W)PAT?/SO
/SY	SY	Synonyms Including Brand Names and Drug Codes ^{1,2}	Segment & Word & Phrase	S AL/SY,DERIV S CO(W)RENITEC/SY
/TC/TN	TC TN	Therapeutic Category ⁶ Brand Name ^{1,2}	Word Segment & Word & Phrase	S CO-RENITEC/SY S ANTIHYPERTENSIVE/TC S AL/TN S LOTRIAL/TN,DERIV S CO-RENITEC/TN

¹ Searchable in the Basic Index and in the Additional Indexes. Any numeric values are searchable in the Basic Index using the (W) operator, e.g. S 143(W)144(W)5/PP

² All chemical names are indexed as complete phrases, individual words, and chemically significant segments of words. Use /FW to restrict retrieval to the complete term, e.g., S ETHANE/FW to only select ethane as a single word rather than as a segment of a larger chemical term, such as trichloroethane.

³ Searchable as /DP in the Basic Index and using DP= or RP= in the Additional Indexes.

⁴ Includes Monograph Name (MN, MN=), C.A. Names (CN, CN=), Brand Names (TN, TN=), Derivative Names (/DERIV), Drug Codes (SY, SY=), and Synonyms (SY, SY=).

⁵ Also /DF.

⁶ Searchable using /TC in the Basic Index and using TC= or TV= in the Additional Indexes.

ADDITIONAL INDEXES

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
AN=	AN	DIALOG Accession Number	Phrase	S AN=03521
AN=	AN	THE MERCK INDEX Monograph Number	Phrase	S AN=03521
BP=	BP	Boiling Point (Celsius) ^{1,7}	Numeric	S BP=223.5
BT=	BP	Boiling Point Text ¹	Word	S BT=DEGREES
CN=	CN	C.A. Chemical Name ¹	Phrase	S CN=S)-1-(N-(1-(ETHOXCARBONYL)?
CO=	CO	Company Name ¹	Phrase	S CO=MERCK & CO?
DN=	DN	Relative Density ^{1,7}	Phrase	S DN=1.0000
DP=	DP	Data Present ^{1,3}	Numeric	S DP=(BOILING POINT AND MELTING POINT)
DT=	DN	Density Text ¹	Phrase	S DT=SUPERCOOLED AND DN=1.0
EC=	MF	Element Count ¹	Word	S EC=(C0020 AND H0028)
FF=	FP	Flash Point (Fahrenheit) ^{1,7}	Numeric	S EC=N0001:N0005
FP=	FP	Flash Point (Celsius) ^{1,7}	Numeric	S FF=84.2
FT=	FP	Flash Point Text ¹	Word	S FP=29
LD=	LD	Lethal Dose (LD50) ¹	Word	S FT=(CLOSED(W)CUP)
ME=	—	Molecular Elements	Word	S LD=(RATS AND S(W)C)
MF=	MF	Molecular Formula	Phrase	S ME=CHNO
MN=	MN	Monograph Name ¹	Phrase	S MF=C20H28N2O5
MP=	MP	Melting Point ^{1,7}	Phrase	S MN=ENALAPRIL
MT=	MP	Melting Point Text ¹	Numeric	S MP=144
MW=	MW	Molecular Weight ⁷	Word	S MT=DEGREES
NA=	NA	Chemical Name ^{1,4}	Numeric	S MW=376.45
OP=	OP	Optical Rotation ^{1,7}	Phrase	S NA=ENALAPRIL
OT=	OP	Optical Rotation Text ¹	Numeric	S OP=10.1:10.9
PN=	PN	Patent Number ¹	Word	S OT=(ALPHA(S)22(S)546)
PP=	PP	Physical Property Information ¹	Phrase	S PN=US 4374829
			Word	S PP=(OFF(W)WHITE AND POWDER)

ADDITIONAL INDEXES (cont'd)

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
RE=	RE	Refractive Index ^{1,7}	Numeric	S RE=1.0:1.5
RI=	RE	Refractive Index Text ¹	Word	S RI=(D(W)20)
RN=	RN	CAS(R) Registry Number	Phrase	S RN=75847-73-3 S RN=75847-73-3/MAIN
RP=	RP	References Present ¹	Phrase	S RP=76095-16-4/DERIV
SO=	SO	Bibliographic Sources ⁶	Word	S SO=PHARMACODYNAMICS
SY=	SY	Synonyms Including Brand Names and Drug Codes ¹	Word & Phrase	S SY=INNOVACE S SO=(FERGUSON(S)(1W)CLIN(W)PHARMACOL?)
TC=	TC	Therapeutic Category ¹	Phrase	S SY="1-(N-(S)-1-CARBOXY-3-PHENYLPROPYL")?
TN=	TN	Brand Name ¹	Word	S TN=ANTIHYPERTENSIVE
TV=	TV	Therapeutic Category (Veterinary) ¹	Phrase	S TV=(ANABOLIC(W)STEROID)
UD=	—	Update	Word	S UD=9999
US=	US	Uses ¹	Phrase	S US=(MORDANT(S)LEATHER)
UT=	UV	Ultraviolet Maximum Text ¹	Word	S UT=ALCOHOL AND UV=235
UV=	UV	Ultraviolet Maximum ^{1,7}	Numeric	S UV=260:265
DISPLAY ONLY				
—	B1	Boiling Point (Derivative)		
—	C1	CA Chemical Name (Derivative)		
—	C2	Company Name (Derivative)		
—	D1	Data Present (Derivative)		
—	D2	Relative Density (Derivative)		
—	FL	Flash Point (Derivative)		
—	L1	Lethal Dose (LD50) (Derivative)		
—	M1	Molecular Composition(Derivative)		
—	M2	Molecular Formula (Derivative)		
—	M3	Melting Point (Derivative)		
—	M4	Molecular Weight (Derivative)		
—	MC	Molecular Composition		
—	N1	Chemical Names (Derivative)		
—	N2	Chemical Names, Additional (Derivative)		
—	O1	Optical Rotation (Derivative)		
—	P1	Physical Property Information (Derivative)		
—	R1	Refractive Index (Derivative)		
—	R2	CAS Registry Number (Derivative)		
—	SB	Bibliographic Sources (Derivative)		
—	SM	Synonyms (Derivative)		
—	T1	Brand Name (Derivative)		
—	UM	Ultraviolet Maximum (Derivative)		

⁷ Numeric values can be entered in several different ways: directly as a number, e.g. S BP=100:0; or in exponential notation, e.g. S BP=1E2. Letter abbreviations are also available: K for thousand; M for million, B for billion, e.g. S BP=0.5K:1.0K. To search a range of values, use a colon between starting and ending value, e.g. S BP=78:79 OR use numeric operators (>, <, >=, and <=), e.g. S 78<=BP<=79.

The Merck Index OnlineSM

File 304

SPECIAL FEATURES

For command descriptions, enter HELP LIMIT, HELP SORT, HELP RANK, HELP MAP online.

LIMIT	/DERIV -- Information relating to the derivative data mentioned in the monograph /MAIN -- Information relating to the main monograph substance data	S S2/DERIV S S1/MAIN
SORT	MF, MN, RN, TC	SORT S2/ALL/MN PRINT S2/5/1-20/TC
RANK	All phrase- and numeric-indexed fields in the Additional Indexes can be ranked. Other RANK codes include: DE	RANK NA RANK BP S4
MAP	MN, NA, PN, RN, SY	MAP RN TEMP S4 MAP SYRN TEMP S3

PREDEFINED FORMAT OPTIONS

NO.	DIALOGWEB FORMAT	RECORD CONTENT
1	--	DIALOG Accession Number
2	--	Full Record, except Literature References and Physical Data
3	Medium	Full Record, except Physical Data
4	--	Full Record
5	--	Full Record
6	Free	DIALOG Accession Number/Monograph Number, Monograph Name, CAS Registry Number, and Molecular Formula
7	Long	Full Record, except Literature References
8	Short	DIALOG Accession Number/Monograph Number, Monograph Name, CAS Registry Number, Molecular Formula, Therapeutic Categories, References Present, Data Present
9	Full	Full Record
K	--	KWIC (Key Word In Context) displays a window of text; may be used alone or with other formats

OTHER OUTPUT OPTIONS

For an explanation, enter HELP TYPE, HELP UDF, HELP TAG online.

USER DEFINED FORMATS	Display codes listed in the Search Options tables can be used to customize output.	TYPE S3/MN, MF, MP, BP/1-10
TAG	Output can be displayed with tags identifying each display field.	TYPE S3/3/1-5 TAG
DIRECT RECORD ACCESS	If the accession number of a specific record is known, it can be used to display the record directly.	TYPE 03521/5 DISPLAY 03521/MN, MF, MP PRINT 03521/9

FOR ONLINE HELP:

See HELP FIELDS 304 for searchable fields; HELP FORMAT 304 for output formats; HELP LIMIT 304 for limits; HELP RATES 304 for cost information; HELP SORT 304 for sorts.

